

Quasiparticle Resonances in the BCS Approach

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Abstract

We present a simple method for calculating the energies and the widths of quasiparticle resonant states. The method is based on BCS equations solved in the Berggren representation. In this representation the quasiparticle resonances are associated to the Gamow states of the mean field. The method is illustrated for the case of neutron-rich nuclei $^{20-22}\text{O}$ and ^{84}Ni . It is shown that the contribution of the continuum coupling to the pairing correlations is small and largely dominated by a few resonant states close to the continuum threshold.

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I. INTRODUCTION

In nuclei close to the drip lines the low-lying excited states belong mostly to the continuum part of the spectrum. It is therefore not surprising that a lot of effort has been devoted recently to the treatment of the continuum in nuclear models.

One of the first attempts to evaluate continuum configurations in nuclei was done within the continuum shell-model (see Ref.[1] and the references therein). In this shell model approach the coupling to the single-particle continuum is introduced through the scattering states of real energies. A different approach for evaluating the continuum processes in the shell-model framework is based on Berggren representation. In this representation the single-particle continuum is formed by a finite number of Gamow resonances and a continuous set of scattering states of complex energy. The advantage of a shell model based on Berggren representation is that it allows a direct calculation of multi-particle resonant states in nuclear systems [2, 3, 4, 5, 6].

The continuum part of the excitation spectrum was also investigated using mean field techniques. One of the most known of these approaches is the continuum-RPA [7, 8]. In this approach, well suited for the description of particle-hole ($p - h$) excitations in closed shell nuclei, the contribution of the continuum to the $p - h$ response function is calculated exactly. To single out from the continuum $p - h$ response the states corresponding to the $p - h$ resonances, a resonant-RPA approach was also developed [9, 10], in which the coupling to the single-particle continuum is introduced through a finite set of Gamow functions.

For even-even nuclei with open shells, where pairing correlations are important, the continuum part of the spectrum corresponds to two-quasiparticle excitations. The unbound two-quasiparticle excitations can be described in the continuum-QRPA approach [11, 12]. Self-consistent continuum-QRPA calculations are presently done only with zero-range forces [12]. At variance with the continuum-RPA, in these calculations the continuum contribution is taken into account only up to an energy cut-off.

In odd-even nuclei the most simple excitations are of the one quasiparticle type. The continuum part of the one quasiparticle spectrum can be calculated by solving the HFB equations with scattering type boundary conditions [13]. By using the behaviour of the phase shift close to a resonance, one can find the quasiparticle resonances of physical interest. The quasiparticle resonances can be found also by solving the HFB equations in complex

energy plane, as have been already done for some particular hamiltonians [14].

However, the simplest framework to evaluate one quasiparticle resonances is the BCS approach. The contribution of resonant states to pairing correlations can be introduced in the BCS equations through the scattering states with energies located in the vicinity of single-particle resonance energies [15, 16, 17]. Alternatively, the resonant continuum was studied by solving the BCS equations in a basis containing only bound and Gamow states [18, 19]. The drawback of this study is that the global quantities associated to the bound state of a nucleus (e.g., binding energy, radii) become complex. The scope of this paper is to show how one can calculate within the BCS approach the energies and the widths of quasiparticle resonances by taking into account the whole contribution of single-particle continuum to pairing correlations and, in the same time, by preserving the correct properties of physical observables.

II. FORMALISM

A. Berggren representation

The quasiparticle spectrum is described here within the Berggren representation. Since this representation is not very common in nuclear structure calculations, we will first describe it briefly, emphasizing those features that we will need in the present paper. For more details see Refs. [20, 21, 22].

The Berggren representation is formed by bound states, Gamow resonances, and a continuous set of scattering states of complex energy. For a given mean field potential (e.g., of Woods-Saxon type), the Gamow states are the outgoing solutions of the Schrodinger equation and correspond to a discrete set of complex wave numbers $k_\nu = \kappa_\nu - i\gamma_\nu$. To each Gamow state $u_{\nu l j}(r)$ with the wave number $k_\nu = \kappa_\nu - i\gamma_\nu$ is associated a "mirror" state $\tilde{u}_{\nu l j}(r)$ with the wave number $\tilde{k}_\nu = -\kappa_\nu - i\gamma_\nu$, such that $\tilde{u}_{\nu l j}^*(r) \equiv u_{\nu l j}(r)$. The Gamow states and their mirrors form a biorthogonal set which can be normalized to unity by using various regularization schemes [20, 23]. All the wave functions written above are the radial single-particle wave functions of angular momentum lj .

The scattering states introduced in the Berggren representation belongs to a contour in the complex momentum or complex energy plane. An example of such a contour in the

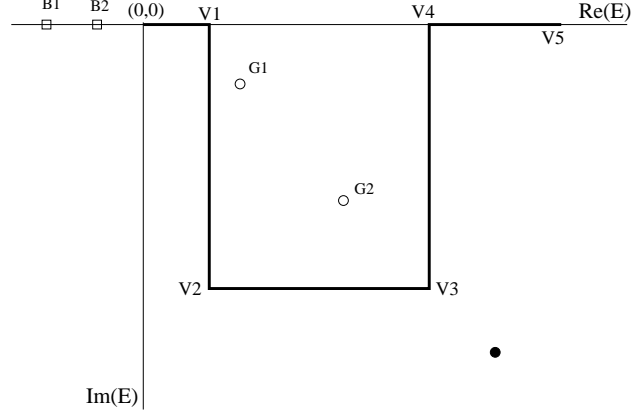


FIG. 1: Contour on the complex energy plane representing the continuum path. The points V_i are the vertices defining the contour. The open circles labelled by G_i indicate the complex energy of the Gamow resonances enclosed by the contour while the open squares label by B_i are the bound states. The dot is a pole of the S-matrix excluded from the Berggren expansion

complex energy plane is shown in Figure 1.

The contour encloses the poles associated to the Gamow states which are taken explicitly into the Berggren representation. The scattering states belonging to the contour, $u_{lj}(\varepsilon, r)$, the enclosed Gamow resonances, $u_{\nu lj}(r)$, and the bound states, $u_{nlj}(r)$, form a complete set, i.e.,

$$\delta(r - r') = \sum_n u_{nlj}(r) u_{nlj}(r') + \sum_\nu u_{\nu lj}(r) u_{\nu lj}(r') + \int_L d\varepsilon u_{lj}(\varepsilon, r) u_{lj}(\varepsilon, r'). \quad (1)$$

In numerical applications the integral along the path L is evaluated by using a finite number of scattering states of energy ε_i defined by a chosen quadrature rule. In what follows this set of scattering wave functions together with the bound and Gamow states are denoted by a unique function, i.e.,

$$\psi_{ilj}(r) = \begin{cases} u_{ilj}(r) & \text{bound states and resonances} \\ \sqrt{\chi_i} u_{lj}(\varepsilon_i, r) & \text{scattering states,} \end{cases}$$

where the quantities χ_i depends on the quadrature. In general, they are defined by $\chi_i = \omega_i \dot{L}_i$, where ω_i are the quadrature weights and \dot{L}_i are the derivative of the complex contour with respect to the parametrisation variable.

In principle, a Berggren representation can be formed by using any set of Gamow states

enclosed by a contour in the complex plane. However, from physical point of view it is better to choose a basis which includes explicitly only narrow Gamow resonances. The contribution of wide resonances which are not included explicitly in the Berggren representation is automatically taken into account through the scattering states belonging to the contour.

B. BCS equations in Berggren representation

The BCS equations in Berggren basis will be derived here from the Hartree-Fock-Bogolubov (HFB) equations in coordinate representation. For zero range forces and for spherically symmetric systems the radial HFB equations have the following form [24]:

$$\begin{pmatrix} h(r) - \lambda & \Delta(r) \\ \Delta(r) & -h(r) + \lambda \end{pmatrix} \begin{pmatrix} U_k(r) \\ V_k(r) \end{pmatrix} = E_k \begin{pmatrix} U_k(r) \\ V_k(r) \end{pmatrix}, \quad (2)$$

where λ is the chemical potential, $h(r)$ and $\Delta(r)$ are the mean field hamiltonian and pairing field, respectively. $U_k(r)$ and $V_k(r)$ are the up and down components of the HFB wave function, denoted below by $|\Psi_k\rangle$. At large distances $U_k(r)$ decays exponentially for $E_k < -\lambda$ and behaves as a scattering state for $E_k > -\lambda$. On the other hand, the function $V_k(r)$ goes to zero exponentially for any value of the quasiparticle energy (for a general discussion on the asymptotic properties of the HFB wave functions see [25]). Consequently, the quasiparticle spectrum is discrete for $E_k < -\lambda$ and continuous for $E_k > -\lambda$. In the ground state of the system the particle density and the pairing density are given by:

$$\rho(r) = \frac{1}{4\pi} \sum_k (2j_k + 1) V_k^*(r) V_k(r) \quad . \quad (3)$$

$$\tilde{\rho}(r) = \frac{1}{4\pi} \sum_k (2j_k + 1) U_k^*(r) V_k(r) \quad . \quad (4)$$

The summations in this equation is over the quasiparticle spectrum of the system (for $E_k > -\lambda$ the sum should be replaced by an integral) up to a given cut-off energy.

In the calculations presented in the next section we take for the mean field a Wood-Saxon potential. The pairing field is calculated self-consistently by using a pairing interaction of the following form [26]:

$$V(\mathbf{r} - \mathbf{r}') = V_0 [1 - \eta (\frac{\rho}{\rho_0})^\alpha] \delta(\mathbf{r} - \mathbf{r}') \equiv V_{eff} \delta(\mathbf{r} - \mathbf{r}'). \quad (5)$$

With this pairing interaction the pairing field is given by:

$$\Delta(r) = \frac{V_{eff}}{2} \tilde{\rho}(r). \quad (6)$$

Before going further with the derivation, it is worth mentioning how the particle and pairing densities behave in excited states belonging to the continuum part of the quasiparticle spectrum of odd-even nuclei. Formally, in order to get the excited state corresponding to a state k of an odd-even nucleus one can simply interchange the eigenvector (U_k, V_k) by (V_k^*, U_k^*) [27]. Consequently, the particle density corresponding to an excited state k will depend on $|U_k|^2$. Thus, if the excited state belongs to the continuum, the function U_k is of a scattering type; hence, there is a finite probability for the particle to be found at infinity, as physically required. On the other hand, by interchanging U_k and V_k one does not affect the asymptotic behaviour of pairing density, which is still going to zero exponentially at very large distances. This is again a physically meaningful condition since when a particle is very far from the nucleus, its contribution to the pairing correlations should vanish.

Starting from the HFB equations in coordinate space we can easily get the HFB equations in Berggren representation. In order to accomplish that, we first expand the HFB wave functions in the Berggren basis:

$$U_k(r) = \sum_i \langle \tilde{\psi}_i | U_k \rangle \psi_i(r) \equiv \sum_i U_{i,k} \psi_i(r) \quad (7)$$

$$V_k(r) = \sum_i \langle \tilde{\psi}_i | V_k \rangle \psi_i(r) \equiv \sum_i V_{i,k} \psi_i(r) \quad , \quad (8)$$

where the expansion coefficients, related to the Bogoliubov transformation, are complex quantities. Then one multiplies the HFB equations from the left with the complex conjugate of a mirror Berggren vector, $\tilde{\psi}_i^*(r)$ and one performs the radial integration. One thus gets the HFB equations in Berggren representation:

$$\begin{pmatrix} \varepsilon_i - \lambda & \Delta_{i,j} \\ \Delta_{i,j} & -\varepsilon_i + \lambda \end{pmatrix} \begin{pmatrix} U_{i,j} \\ V_{i,j} \end{pmatrix} = E_i \begin{pmatrix} U_{i,j} \\ V_{i,j} \end{pmatrix}, \quad (9)$$

which formally have the same structure as in any hermitic representation. The essential difference is that the matrix elements of the pairing field are defined with the Berggren metric, i.e., by using mirror states in the bra positions and employing regularisation techniques for

calculating the diverging integrals. Thus, $\Delta_{i,j}$ is defined by:

$$\Delta_{i,j} = \langle \tilde{\psi}_i | \Delta(r) | \psi_j \rangle = \int dr r^2 \psi_i(r) \Delta(r) \psi_j(r) , \quad (10)$$

where $\tilde{\psi}_i$ is the mirror state corresponding to ψ_i .

Finally, from Eq. (9) one can get the BCS equations in the Berggren representation by neglecting the off-diagonal matrix elements of the pairing gap matrix. Physically, this approximation means that one neglects the pairing correlations associated to the Cooper pairs formed in states which are not time-reversed. In this approximation the expansions (7,8) of the HFB wave function are reduced to one term. The corresponding expansion coefficients, denoted below by u_i and v_i , are complex quantities. They satisfy the condition $u_i^2 + v_i^2 = 1$, which is obtained from the Berggren normalization condition of the HFB wave function Ψ_i , i.e., $\langle \tilde{\Psi}_i | \Psi_i \rangle = 1$. By combining this condition with Eq.(9) one gets the BCS equations in the Berggren representation:

$$v_i^2 = \frac{1}{2} \left(1 - \frac{\varepsilon_i - \lambda}{E_i} \right) \quad (11)$$

$$E_i = \sqrt{(\varepsilon_i - \lambda)^2 + \Delta_i^2} \quad (12)$$

where

$$\Delta_i = \int dr r^2 \psi_i^2(r) \Delta(r) \quad (13)$$

and the chemical potential is found from the particle number equation:

$$N = \int \left[\sum_i (2j_i + 1) v_i^2 \psi_i^2(r) \right] r^2 dr . \quad (14)$$

In conclusion, apart from the radial integrals which are calculated with the Berggren metric (and a given regularisation procedure), the BCS equations in the Berggren representation have formally the same expression as in any hermitic and discrete basis. However, one should keep in mind that the pairing gaps and the occupation probabilities associated to the scattering states correspond to an energy interval.

The advantage of working in Berggren representation is that the quasiparticle resonances appear as unique states, associated to the Gamow functions. In this way the widths of the quasiparticle resonances, given by the imaginary parts of the quasiparticle energies, are calculated unambiguously.

In principle, one can get the complex energies associated with the resonant states by solving the BCS equations in complex energy plane. However, due to the strong non-linearity of the BCS equations, this is a difficult numerical task. One can avoid this task by using the fact that the pairing field and the chemical potential do not depend on the representation. Thus, they can be calculated by solving the BCS equations in a real energy representation, which can be obtained by choosing the L contour to be the real energy axis. From the pairing field calculated using the real energy axis, we can then get, by using Eq.(11c), the pairing gaps associated to the Gamow states. With these values of the pairing gaps, which are complex quantities, one can finally calculate, by using Eq.(11b), the energies of the resonant quasiparticle states.

III. APPLICATIONS

The scope of the calculations presented below is twofold: a) to illustrate, within the approximation discussed above, how the energies and the widths of quasiparticle resonant states behaves in neutron-rich nuclei; b) to analyse what is the relative contribution of resonant and non-resonant continuum upon pairing correlations in nuclei close to the dripline. For these purposes we have performed calculations for the isotopes $^{20-22}\text{O}$ and ^{84}Ni .

A. Mean fields and single-particle states

The BCS calculations presented in this section are based on a mean field of Woods-Saxon form. In addition to the mean field, we take also a standard spin-orbit interaction, with the form factor given by the derivative of a Wood-Saxon function. The Wood-Saxon parameters we used for oxygen isotopes have the following values: $V_0=55.8$ MeV, $V_{so}=12.12$ MeV, $r_0=1.21$ fm and $a = 0.65$ fm. The values of r_0 and a are the same for the mean field and for the spin-orbit interaction. With these parameters we get for the isotope ^{17}O the single-particle energies shown in Table I.

One can notice that the energy of the single-particle state $d_{3/2}$ is very close to the experimental value, equal to $(0.94 - i0.05)$ MeV [28] . The relevant single-particle resonances in oxygen isotopes are the states $2d_{3/2}$ and $1f_{7/2}$. The corresponding complex energies shown in Table I are the energies of the Gamow states, i.e., $\varepsilon_\nu = \epsilon_\nu - i\Gamma_\nu/2$, where Γ_ν is the width

TABLE I: Single- particle energies (in MeV) corresponding to ^{17}O and ^{79}Ni

^{17}O		^{79}Ni	
State	Energies	State	Energies
$1f_{7/2}$	7.45-i 1.53	$1h_{11/2}$	3.56-i 0.02
$1d_{3/2}$	0.91-i 0.05	$1g_{7/2}$	1.93-i 0.01
$2s_{1/2}$	-3.26	$2d_{3/2}$	0.51-i 0.06
$1d_{5/2}$	-4.12	$3s_{1/2}$	-0.82
$1p_{1/2}$	-14.57	$2d_{5/2}$	-1.44

of the resonance.

For the isotope ^{84}Ni we have chosen the following Wood-Saxon parameters: $V_0=42.0$ MeV, $V_{so}=16.0$ MeV, $r_0=1.27$ fm and $a = 0.67$ fm. As in the previous case, the values of r_0 and a are the same for the mean field and for the spin-orbit interaction. The single-particle states corresponding to the major shell $N=50-82$ are given in Table I. It can be seen that at variance to the situation in stable nuclei (e.g., tin isotopes) the states $1d_{3/2}$, $1g_{7/2}$ and $1h_{11/2}$ are not bound states but single-particle resonances. In the presence of pairing correlations these states will generate the quasiparticle resonances discussed in the subsection C.

B. The BCS solution: contribution of resonant continuum

With the single-particle states described in the previous section we have solved the BCS equations for the pairing force given by Eq.(5). For the parameters of the pairing force we have used the following values: a) oxygen isotopes: $V_0=-456$ MeV fm $^{-3}$, $\eta=1$, $\alpha=1$; b) nickel isotope: $V_0=-1130$ MeV fm $^{-3}$, $\eta=1$, $\alpha=1$. In both cases we have introduced in the calculations all the bound states. In order to analyse various approximations of continuum treatment, we have performed two types of BCS calculations.

First, we have considered in the BCS equations the whole contribution of the continuum states up to a cut-off energy equal to 10 MeV. The continuum contribution is introduced through the scattering states of real energy. The number of scattering states per energy interval was increased, especially in the region of single-particle resonances, up to the convergence. In the calculations we have considered for the continuum states the same (lj)

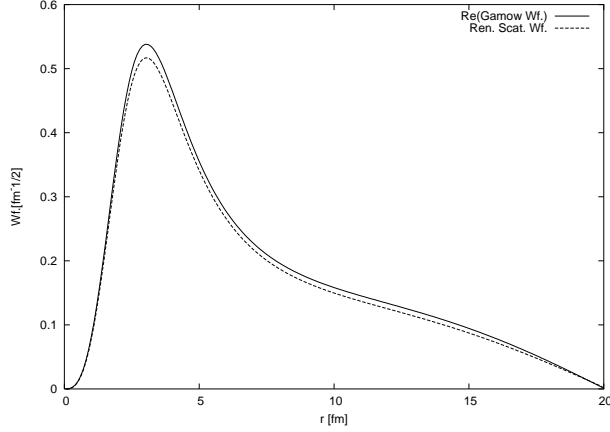


FIG. 2: The scattering state $d_{3/2}$ evaluated at the position of the $1d_{3/2}$ resonance, i. e. 0.910 MeV (full line). The dashed line shows the real part of the corresponding Gamow function, with the energy equal to (0.910,-0.050) MeV.

TABLE II: Average gap, pairing energies (in MeV) and root-mean-square radii (in fm) calculated by using the representations discussed in the text.

	cBCS			rBCS			bBCS		
	$\langle \Delta \rangle$	E_p	$\langle r \rangle$	$\langle \Delta \rangle$	E_p	$\langle r \rangle$	$\langle \Delta \rangle$	E_p	$\langle r \rangle$
^{20}O	1.831	-1.044	2.916	1.800	-1.013	2.913	1.784	-1.002	2.912
^{22}O	1.412	-0.876	3.040	1.384	-0.856	3.038	1.370	-0.849	3.038
^{84}Ni	1.493	-0.644	4.650	1.390	-0.610	4.647	1.386	-0.606	4.646

values as for the bound states. These calculations are called below continuum-BCS (cBCS).

In the second BCS calculation we have kept from the continuum only the contribution corresponding to the resonant states. More precisely, we have included in the calculations only the scattering states with the energies in the interval $\varepsilon_\nu \pm 2\Gamma_\nu$, where ε_ν and Γ_ν are the energies and the widths of the resonances given in Table I. These calculations are referred to as resonant-BCS (rBCS) [16].

The results of these two calculations are shown in Table II. In order to see what is the total contribution of the continuum, in Table II we give also the results obtained when in the calculations we include only the bound states (bBCS).

From Table II one can first notice that for all the isotopes analysed here the contribution of the continuum to the correlation energies is rather small. Secondly, one can see that

the contribution of the continuum is essentially given by a few low-lying single-particle resonances. In the presence of pairing correlations they generate the resonant quasiparticle states, analysed in the next subsection.

C. Quasiparticle resonances

The quasiparticle resonances, which describe unbound excited states in odd-even nuclei, are obtained from the BCS equations written in Berggren representation. In this representation each quasiparticle resonance is described by a unique state, corresponding to a single-particle Gamow state. This is different from the case of real energy representations, where a quasiparticle resonance is characterized by a continuous set of scattering states with energies in the vicinity of the resonance energy.

As it was already discussed in the previous section, in order to get the energies and the widths of the quasiparticle resonances is necessary to calculate the pairing field and the chemical potential. Since these two quantities do not depend on the representation, we can calculate them by solving the BCS equations by using a real energy representation. Thus, we have solved the BCS equations by using all the bound states and the whole contribution of the continuum states up to a cut-off energy equal to 10 MeV. The continuum contribution was introduced through the scattering states of real energy. This calculation corresponds to the case cBCS described in the previous subsection.

With the mean field and the chemical potentials provided by the cBCS equations we then calculated, by using Eqs.(11c), the pairing gaps associated to a Gamow state and the corresponding quasiparticle energies and widths. The results are shown in Table III. From these results one can see clearly how the widths of single-particle resonances are changing by the pairing correlations. This direct access to the widths of quasiparticle resonances is the main advantage of expressing the BCS solution in terms of single-particle Gamow functions.

IV. SUMMARY AND CONCLUSIONS

In this paper we have discussed how the energies and the widths of quasiparticle resonances can be calculated by using the BCS equations written in Berggren representation.

TABLE III: The quasiparticle energies, E_i , the corresponding single-particle energies measured from the chemical potential, i.e., $\epsilon_i = |\varepsilon_i - \lambda|$ and the occupation probabilities. The energies are in MeV.

State i	^{20}O			^{22}O			State i	^{84}Ni		
	ϵ_i	E_i	v_i^2	ϵ_i	E_i	v_i^2		ϵ_i	E_i	v_i^2
$1d_{5/2}$	(0.301,0)	(1.656,0)	(0.591,0)	(1.060,0)	(1.657,0)	(0.820,0)	$2d_{5/2}$	(1.255,0)	(1.720,0)	(0.864,0)
$2s_{1/2}$	(0.564,0)	(1.301,0)	(0.283,0)	(0.195,0)	(1.020,0)	(0.596,0)	$3s_{1/2}$	(0.631,0)	(1.044,0)	(0.801,0)
$1d_{3/2}$	(4.736,-0.141)	(4.878,-0.084)	(0.015,-0.003)	(3.977,-0.148)	(4.082,-0.075)	(0.013,-0.003)	$2d_{3/2}$	(0.701,-0.050)	(1.050,-0.183)	(0.171,-0.030)
$1f_{7/2}$	(11.273,-1.528)	(11.310,-1.574)	(0.002,-0.001)	(10.514,-1.528)	(10.541,-1.559)	(0.001,-0.001)	$1f_{7/2}$	(2.121,-0.010)	(2.486,-0.021)	(0.073,-0.002)
							$1h_{11/2}$	(3.745,-0.018)	(3.937,-0.025)	(0.024,-0.001)

In this representation the pairing gaps associated to the quasiparticle resonances, Δ_ν , are obtained by integrating the pairing field with the square of Gamow states. On the other hand, the pairing field, which does not depend on representation, is calculated by solving the BCS equations in a single-particle basis formed from bound states and scattering states of real energies. Then, the energies associated to the quasiparticle resonances E_ν are calculated by using the standard BCS formula, i.e., $E_\nu = \sqrt{(\epsilon_\nu - \lambda)^2 + \Delta_\nu^2}$, where ϵ_ν are the energies of the Gamow states. Since both ϵ_ν and Δ_ν are complex quantities, the quasiparticle energies are also complex. As in the case of single-particle resonances, the imaginary parts of E_ν are associated to the widths of the quasiparticle resonances.

The calculation of quasiparticle resonances was illustrated for the case of the isotopes $^{20-22}\text{O}$ and ^{84}Ni . It was shown that in these isotopes the contribution of the single-particle resonant states upon pairing correlations is dominant compared to the contribution of background continuum. The most relevant aspect of the BCS calculations presented here is that they describe the excitations in resonant quasiparticle states in term of individual states, as in the case of bound states excitations.

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